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ABSTRACTS

of contributions to the

21st International NTZ-Workshop on

New Developments in Computational Physics

CompPhys20

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Preface

Welcome to the 21st International NTZ-Workshop *CompPhys20* on *New Developments in Computational Physics*. As in previous years, also this year's Workshop will cover a broad spectrum of different fields ranging from general aspects of computational and statistical physics over computer simulation studies in condensed and soft matter physics, including applications to biological systems, and random networks to the intriguing properties of quantum systems and high-energy physics. Following the traditional setup of the Workshop, it is also this year designed to provide a forum for an informal exchange of ideas and to meet – due to the Covid-19 pandemic for the first time virtually – in a relaxed atmosphere "in Leipzig" at the beginning of Christmas time.

The main part of the Workshop takes place from 03 – 04 December 2020 in a "Zoom Lecture Hall" (talks) and a "Gather Town" (posters and coffee breaks). As in previous years, the Saturday, 05 December 2020, is devoted to various discussion rounds and collaborative meetings which will take place in the "Gather Town".

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Doctoral College "$\mathbb{L}^4$" of Deutsch-Französische Hochschule (DFH-UFA), DFG Collaborative Research Centre SFB/TRR 102 "Polymers under Multiple Constraints", Research Academy Leipzig (RALeipzig), and Leipzig Graduate School of Natural Sciences "BuildMoNa".

Leipzig,
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Wolfhard Janke

Abstracts

Applying simulated annealing to telescope phasing

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Based on an analogy between a multimirror optical device (telescope or microscope etc) and the Solid-On-Solid (SOS) model, simulated annealing is a logical algorithm to invoke in order to achieve optical flatness in these devices. In this presentation I will review our 2 decades of study of such models and then ask "but is this algorithm the only/best one?". A simple steepest descent has also been used but can lead to local, not global minima but perhaps other algorithms will perform as well or better than simulatd annealing. The presentation will hopefully lead to proposals from the audience for other possible algorithms.

Domain-growth kinetics of two-dimensional long-range Ising model at low temperatures

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In this talk, I will discuss the low-temperature domain-growth kinetics of long-range Ising model with power-law exchange-coupling in dimension $d = 2$. I will describe both the multi-domain systems and the simplified models in order to precisely determine domain-growth exponent at temperature $T = 0$.

Infinite disorder fixed point of the 2D and 3D disorder quantum Potts models

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The random quantum Potts model is considered on hypercubic lattices in dimensions 2, and 3 using the numerical implementation of the Strong Disorder Renormalization Group introduced by Kovacs and Iglói. The critical exponents are estimated for several numbers of states q. In contrast to what is observed in dimension $d = 1$, a dependence of the critical exponents with q is observed for $d > 1$.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration

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We present a physical interpretation of machine learning functions, opening up the possibility to control properties of statistical systems via the inclusion of these functions in Hamiltonians. In particular, we include the predictive function of a neural network, designed for phase classification, as a conjugate variable coupled to an external field within the Hamiltonian of a system. Results in the two-dimensional Ising model evidence that the field can induce an order-disorder phase transition by breaking or restoring the symmetry, in contrast

with the field of the conventional order parameter which can only cause explicit symmetry breaking. The critical behaviour is then studied by proposing reweighting that is agnostic to the original Hamiltonian and forming a renormalization group mapping on quantities derived from the neural network. Accurate estimates of the critical fixed point and the operators that govern the divergence of the correlation length are provided. We conclude by discussing how the method provides an essential step towards bridging machine learning and physics.

Efficient calculation of the divided differences of the exponential function

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We introduce a method for calculating the divided differences of the exponential function by means of addition and removal of items from the input list to the function. Our technique exploits a new identity related to divided differences recently derived by F. Zivcovich [Dolomites Research Notes on Approximation 12, 28–42 (2019)]. We show that upon adding an item to or removing an item from the input list of an already evaluated exponential, the re-evaluation of the divided differences can be done with only $O(sn)$ floating point operations and $O(sn)$ bytes of memory, where $[z_0, \ldots, z_n]$ are the inputs and $s \propto \max_{i,j} |z_i \pm z_j|$. We demonstrate our algorithm's ability to deal with input lists that are orders-of-magnitude longer than the maximal capacities of the current state-of-the-art. We discuss in detail one practical application of our method: the efficient calculation of weights in the off-diagonal series expansion quantum Monte Carlo algorithm.

How do clusters in phase-separating active matter systems grow? A study for systems containing active Brownian particles (P)

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Via computer simulations we study morphology and growth in a system containing active Brownian particles. The overlap-preventing passive interaction between two active particles has been taken care of via a variant of the Lennard-Jones potential. We have worked with low overall density of particles that give rise to disconnected clusters. The growth of these objects has been accurately quantified and compared with corresponding results from systems containing Vicsek-like active particles.

Spreading processes in "post-epidemic" environments

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We analyze infection spreading processes in a system where only a fraction p of individuals can be affected by disease, while remaining $1 - p$ individuals are immune. Such a picture can emerge as a natural consequence of previously terminated epidemic process or arise in formerly vaccinated population. To this end, we apply the synchronous cellular automata algorithm studying stationary states and spatial patterning in SI, SIS and SIR models on a square lattice with the fraction p of active sites. A concept of "safety patterns" of susceptible agents surrounded by immune individuals naturally arises in a proposed system, which plays an important role in the course of epidemic processes under consideration. Detailed analysis of distribution of such patterns is given, which in turn determine the fraction of infected agents in a stationary state. Estimates for the threshold values of the basic reproduction number as a function of active agents fraction p are obtained as well. In particular, our results allow to predict the optimal fraction of individuals, needed to be vaccinated in advance in order to get the maximal values of unaffected agents in a course of epidemic process with a given curing rate.

Lattice scalar electrodynamics with noncompact gauge fields

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We study a noncompact lattice formulation of the three-dimensional electrodynamics with N-component complex scalar fields (lattice Abelian-Higgs theory). For N larger than 1 this model presents a phase diagram with three different phases, associated to the different large distance behaviour of scalar and gauge correlations: the Coulomb phase (short-ranged scalar and long-ranged gauge correlations), the Higgs phase (condensed scalar-field and gapped gauge correlations), and the molecular phase (condensed scalar-field and long-ranged gauge correlations). These phases are separated by transition lines whose nature depends on the phases they separate and on the number N of components of the scalar field: the Coulomb-to-molecular transition line (where gauge correlations are irrelevant) is associated with the Landau-Ginzburg-Wilson theory sharing the same SU(N) global symmetry but without explicit gauge fields. On the other hand, the Coulomb-to-Higgs transition line (where gauge correlations are relevant) turns out to be described by the continuum Abelian-Higgs field theory with explicit gauge fields: these transitions are indeed second order for N large enough, and the critical exponents extracted from our numerical simulations agree for $N = 15$ and 25 with the renormalization-group predictions of continuum Abelinan-Higgs field theory.

Evolutionary spatial games with mean-field interactions

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We introduce a mean-field term to an evolutionary spatial game model. Namely, we consider the game of Nowak and May, based on the Prisoner's dilemma, and augment the game rules by a mean-field term. This way, an agent operates based on both local information from its neighbors and non-local information via the mean-field coupling. We simulate the model and construct the steady state phase diagram, which shows significant differences due to the mean-field term.

Fractality and persistence during zero-temperature coarsening in the 2D long-range Ising model

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We investigate the nonequilibrium dynamics following a quench to zero temperature of the Ising model with power-law decaying long-range interactions and provide estimates of the nonequilibrium exponents, viz., the growth exponent α, the persistence exponent θ, and the fractal dimension d_f. It is found that the growth exponent is independent of the interactions. The fractal dimension of the nearest-neighbor Ising model is recovered for interactions in the short-range like regime, while the other exponents differ significantly. For the system to achieve this, the persistence exponent is observed altered accordingly to $d - d_f = \theta/\alpha$. This relation has been previously proposed for annihilation processes and later numerically tested for the nearest-neighbor Ising model.

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Aging dynamics following quenches of Ising model from critical points to the ordered regions (P)

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Following quenches of initial configurations having long range spatial correlations, prepared at the demixing critical points, we have studied the aging phenomena in Ising model via Monte Carlo simulations in space dimensions $d = 2$ and $d = 3$. We obtained results for the decay of the order- parameter autocorrelation function and the corresponding power-law exponents for both conserved and nonconserved (order-parameter) dynamics of the model. In a given dimension, these numbers appear to be same for both the cases. These results are drastically different from those for quenchesfrom infinite temperature. Our results satisfy certain bounds.

A simple analytical description of spread of communicable diseases

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We study real data on the spread of COVID-19 in various countries. There exist two regimes, as is well known. Early time growth in the number of infections is exponential. Due to natural reasons as well as imposed social restrictions the spread is slower at late time. This is analogous to finite-size effects in kinetics of phase transitions. Via appropriate formulation of finite-size scaling we investigate universal features in the infection rate. Via this approach we also derive a simple analytical function that describes the disease dynamics quite accurately in many countries, combining both exponential and post-exponential periods of a wave. The model as a whole is predictive in nature. We believe that the outcome of this study will be of relevance in more general context.

Large-deviations of the SIR model

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Not only due to the current COVID-19 pandemic, research in disease spreading is a well studied topic in interdisciplinary science. Here we investigate the standard susceptible-infected-recovered (SIR) model on small-world networks with given initial conditions. We are particularly interested in the phase where an outbreak (per time unit) is very unlikely, while the model is still close to the epidemic transition. This regime is of particular interest, because for even lower infection rates, basically no outbreak will ever occur, thus the disease is like not existing. On the other hand, beyond the epidemic transition, a disease will have occurred already a long time ago and typically almost all people are immune, i.e., such a virus of will actually not be regarded as a threat. Thus, the regime of rare outbreaks is most interesting. We are able to investigate this regime by using special large-deviation techniques. We study the probability density functions of the cumulative number C of infections and the maximum M of the number of currently infected people down to very small probabilities like 10^{-2000}. We also measure correlations with other measurable quantities to identify reasons for the occurrence of outbreaks.

Computer simulations of selective adsorption and chemical reaction of NOx from air by two porous materials (P)

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The poisoned air pollutions nitrogen oxides (NOx) exist only in permanent chemical reaction. Their separation

from air can be done by selective adsorption on microporous materials. This can be investigated by a combination of Gibbs Ensemble Monte Carlo (GEMC) and Reactive Monte Carlo (RxMC) simulations. In this paper the porous materials MIL-127 and a Carbon Nanotube (CNT) are considered. Very high selectivities of several hundred up to more than 1000 could be found.

Evidence for supersymmetry in the random-field Ising model at five dimensions

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We provide a nontrivial test of supersymmetry in the random-field Ising model at five spatial dimensions, by means of extensive zero-temperature numerical simulations. Indeed, supersymmetry relates correlation functions in a D-dimensional disordered system with some other correlation functions in a $D-2$ clean system. We first show how to check these relationships in a finite-size scaling calculation and then perform a high-accuracy test. While the supersymmetric predictions are satisfied even to our high accuracy at $D=5$, they fail to describe our results at $D=4$.

Simulation of extremely rare ultra-fast non-equilibrium processes close to equilibrium

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Work theorems like Crooks equation allow to obtain equilibrium quantities from non-equilibrium processes. A standard setup is starting a system in contact to a heat bath in equilibrium, then executing a process by changing some external parameter which leads to performing work, and ending in some non-equilibrium configuration. The distribution $P(W)$ of the work allows to extract the free energy difference ΔF between equilibrium starting state and the imaginary final equilibrium state, which would be obtained if one waited long enough after the process has been finished. The region of $P(W)$ which is most relevant to obtain ΔF is where $W \approx \Delta F$. Nevertheless, if the investigated system is not too small, $P(W)$ will be tiny, like 10^{-15} or smaller, being located in the rare-event tail. Thus, when studying such processes by simulation, one needs to use large-deviation approaches applied to the dynamic evolution of the respective model. Here we will investigate the question how similar non-equilibrium processes are to the equilibrium ones beyond comparing a scalar number like the work. Still, we study this question as a function of the measured work W. For that purpose we investigate numerically the unfolding and refolding of RNA secondary structures under influence of an external force f. Fortunately, for this model the equilibrium behavior can be accessed exactly by dynamic programming algorithms allowing to sample equilibrium unfolding and folding processes. We compare between equilibrium and non-equilibrium dynamics by means of force-extension curves $n(f)$ and overlap profiles $\sigma(f)$. Our results indicate that indeed the extreme low-probability trajectories which exhibit $W \approx \Delta F$, and thus contribute most to the determination of ΔF via Crooks equation, are most similar to the equilibrium trajectories.

Ring polymers on percolation clusters

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In the present work, the cyclic polymer chains (rings) in structurally disordered environment (e.g. in the cross-linked polymer gel) are studied exploiting the model of closed self-avoiding walks (SAWs) trajectories on $d=3$-dimensional percolation clusters. Numerical simulations with an application of pivot algorithm are performed. The estimates for the universal size and shape characteristics such as size ratios, averaged asphericity and prolateness

of typical polymer conformation are obtained. Our results quantitatively describe an elongation and increase of anisotropy of ring polymers in disordered environment comparing with the pure solvent.

Distribution of the excitations of the random quantum Ising chain: Comparison with extreme statistics

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The excitation energy (ε) of the random transverse Ising chain is calculated numerically and by the strong disorder RG method at the disordered Griffiths phase. In a large finite chain of length L the distribution of the first gap, $P(\varepsilon, L)$, can be well fitted by a Fréchet extreme form, $P_{Fr}[\varepsilon, z(L)]$ with an effective dynamical exponent $z(L)$, which approaches the true exponent, z, as $z - z(L) \sim \ln^{\omega} L/L$, with $\omega > 1$, which slowly varies with distance from the critical point. The finite-size corrections to the extreme distribution are found to scale as: $P(\varepsilon, L) - P_{Fr}[\varepsilon, z(L)] \approx \ln^{\omega} L/L p_1(\varepsilon L^{z(L)})$, where the correction term, $p_1(x)$ is different from the one, which has been calculated for independent and identically distributed random variables.

How to control a cooperative co-infection dynamics

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In previous studies, it has been shown that a cooperative interaction in a co-infection spread can lead to a first order transition at a decreased threshold. Here, we are investigating how interventions like quarantine or vaccinating with certain rates can turn the first order transitions into the second order ones while increasing the threshold. We have used symmetric double Susceptible-Infectious-Recovered (SIR) equations to model the dynamics of co-infections spreading among a well-mixed population. Then we have intervened the epidemic dynamics by decreasing the susceptible population at a given rate, which means that the decreased block will be either quarantined or added directly to the immune block at the same rate. First, we have solved the equations numerically for a wide range of parameters and different initial conditions. We have illustrated how these interventions can change the type of the transition when the outflow rate gets large enough. Second, we have also solved the equations analytically for a special case in which the outflow rate varies with the size of the infectious block. Using the exact results for this special case, we have been able to investigate how characteristics of the fixed points change when the parameters change.

Some interesting results on random-field Potts model

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I will talk on some interesting findings on ground states and critical properties of a three-state random-field Potts model, obtained through extensive numerical work.

Influence of polymer chain knotting on monomer density in a slit of two parallel walls (P)

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Dilute polymer solution in confined geometries can present interesting behaviour due to entropic reasons [1, 2, 3, 4]. Their properties can be altered by changing temperature, geometry of surfaces or topological structure of polymers, which has the effect on the type and magnitude of interaction between polymer itself and environemnt – walls, colloidal particles etc. Polymers, long and flexible like in coil phase, have high probability to self entangle. The higher degree of entanglement the more they are tight up and movements of single mers are constrained (less degrees of freedom is left for parts of polymer to move). On the other hand, polymer solutions under confinement can present interesting features like arising of depletion forces [2, 3, 5, 6]. Taking those properties into account it is interesting to investigate the behavior of ring polymer chains with topologically different entanglements in confined geometries like slit with mixed interactions arising between polymer and surrounding walls. We performed molecular dynamics simulations obtaining results for the monomer density profiles for linear polymers and ring polymer chains of $N = 360$ monomers with different topological entanglements like: 0 1, 3 1, 6 1, 7 1 and 9 1 or twisted knots with number of twists equal ten and twenty. We show that differences in those polymer structures influence the radius of gyration and monomer density profiles in the slit for range of temperatures – from 1.00 to 3.00 in reduced units.

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Rebound suppression of a droplet impact on a supersolvophobic surface by a small amount of polymer additives

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A small amount of polymer dissolved in a droplet suppresses droplet rebound when it impinges on a supersolvophobic surface. This work investigates impacting dynamics of a droplet of dilute polymer solution depending on the molecular weight and the concentration of the polymer by using multi-body dissipative particle dynamics simulations. Either the longer polymer or the high polymer concentration suppresses rebound of a droplet although its shear viscosity and the liquid-vapor surface tension are not different from those of a pure solvent droplet. We found a new mechanism of the anti-rebound in which the resistance is applied against the hopping motion, while behavior of the non-rebounding droplet at the earlier spreading and retraction stages is same as for the rebounding droplets. Two polymer contributions to reducing the rebound tendency are quantitatively analyzed: the alteration of the substrate wettability by the polymer adsorption and the polymer elongation force.

Ordering behavior of the two-dimensional Ising spin glass with long-range correlated disorder

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The standard two-dimensional Ising spin glass does not exhibit an ordered phase at finite temperature. Here, we investigate if long-range correlated bonds can have an influence on this characteristic. Therefore, the bonds are drawn from a Gaussian distribution with a two-point correlation for bonds at distance r that decays as $(1+r^2)^{-a/2}$,

$a \geq 0$. To see how this influences the ordering behavior we study numerically the ground state and domain wall excitations. The results indicate still the absence of spin-glass phase at any finite temperature. A further analysis reveals that the correlation has strong effects on local length scales inducing ferro/antiferromagnetic domains into the system. The length scale of ferro/antiferromagnetic order diverges exponentially as the correlation exponent approaches a critical value, $a \to a_{\text{crit}} = 0$. Thus, our results suggest that the system becomes a ferro/antiferromagnet only in the limit $a \to 0$.

Boundary critical behavior of the three-dimensional Heisenberg universality class

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We study the boundary critical behavior of the three-dimensional Heisenberg universality class, in the presence of a bidimensional surface. By means of high-precision Monte Carlo simulations of an improved lattice model, where leading bulk scaling corrections are suppressed, we prove the existence of a special phase transition, with unusual exponents, and of an extraordinary phase with slowly-decaying correlations. These findings contrast with naïve arguments on the bulk-surface phase diagram, and allow to explain some recent puzzling results on the boundary critical behavior of quantum spin models.

Modeling structure formation of twin polymerization

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Twin polymerization is a recently developed complex reaction mechanism where organic-inorganic twin monomers react to a nanoporous hybrid material consisting of highly interweaved organic and inorganic networks of domain sizes in the range of 2.5 to 5 nm. In order to get an in-depth understanding of the occurring structure formation process several modeling approaches, i.e. DFT calculations, molecular dynamics simulation or bond fluctuation approaches have been applied. Here, we will show how different model parameters, as reaction probabilities, movability, or attraction of the twin monomers influence structural properties of the final hybrid material, as specific surface area or local porosity distribution. Hereby, we point out which implications theses parameter changes have on the underlying chemical structure. and we can identify key factors to adapt structural properties to fulfill desired requirements for possible applications.

Adsorption of 2d polymers with two- and three-body self-interactions

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Using extensive Monte Carlo simulations, we investigate the surface adsorption of self-avoiding trails on the triangular lattice with two- and three-body on-site monomer-monomer interactions. In the parameter space of two-body, three-body, and surface interaction strengths, the phase diagram displays four phases: swollen (coil), globule, crystal, and adsorbed. For small values of the surface interaction, we confirm the presence of swollen, globule, and crystal bulk phases. For sufficiently large values of the surface interaction, the system is in an adsorbed state, and the adsorption transition can be continuous or discontinuous, depending on the bulk phase. As such, the phase diagram contains a rich phase structure with transition surfaces that meet in multicritical lines joining in a single special multicritical point. The adsorbed phase displays two distinct regions with different characteristics, dominated by either single or double layer adsorbed ground states. Interestingly, we find that there is no finite-temperature phase transition between these two regions though rather a smooth crossover.

Collective effects of the cost of opinion change

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We study an opinion dynamics model, where an agent i with opinion $x_i(t)$ can be influenced by the opinions of all agents whose opinions are similar, i.e., in the range $[x_i - \varepsilon_i, x_i + \varepsilon_i]$. We extend this well known Hegselmann-Krause model by introducing a cost, which has to be payed each time an agent changes its opinion. The model without cost already shows complex behavior for different choices of ε_i, in regards of the ability of the society to reach a common consensus opinion, or to fragment into many small groups with different opinions. For our extension with costs we find for some choices to assign the ε_i a critical cost, above which the simulated society loses the ability to reach consensus. We determine the corresponding critical exponents of this second-order phase transition.

Ising model on the foam

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We propose an algorithm for the foam generation in the plane. The foams are sparse and rigid structures with a minimal density a hundred times lighter than the regular lattice. We place Ising spins on the foam and look for the thermodynamic observables. There is a transition from the one-dimensional behavior to the two-dimensional random Ising model behavior. The simulated magnetic properties resemble those observed in experiments with the palladium foams. We present an analysis of the physical length relations among which defines different behavior of the model. The preliminary results of simulations demonstrate the validity of our analysis.

Using radial distribution function (RDF) in search of structural water around biopolymeric structures (P)

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Water, that is so common in our environment and that is an essential component of our life, is an object of interest for researchers for centuries. Some of its physicochemical properties are extraordinary. Although water is a liquid, many experimental studies indicate that under certain conditions water has the characteristics of an ordered structure. Using a tool called radial distribution function to analyze molecular dynamics simulation results we try to answer whether the water in the considered systems shows features of an ordered structure.

Growth of fractal clusters in a single component Lennard-Jones system (P)

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We study kinetics of phase separation in a single component Lennard-Jones system, via molecular dynamics simulations, in space dimension $d = 3$, at low density regime inside the coexistence curve. At very low temperature, disconnected fractal clusters form. These objects are crystalline in nature and move ballistically in the vapor background. We study the temperature dependence of growth and fractality of these clusters. The quantitative outcomes are discussed in the background of a simple theory of ballistic aggregation.

Universality in the three-dimensional random bond quantum Heisenberg antiferromagnet

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The three-dimensional quenched random bond diluted (J_1-J_2) quantum Heisenberg antiferromagnet is studied on a simple-cubic lattice. Using extensive stochastic series expansion quantum Monte Carlo simulations, we perform very long runs for $L \times L \times L$ lattice up to $L = 48$. By employing standard finite-size scaling method, the numerical values of the Néel temperature are determined with high precision as a function of the coupling ratio $r = J_2/J_1$. Based on the estimated critical exponents, we find that the critical behavior of the considered model belongs to the pure classical $3D$ $O(3)$ Heisenberg universality class.

Tunning exchange bias in inverted antiferromagnetic/ferromagnetic core/shell nanoparticles by binary alloy shells

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We investigate exchange bias properties of an inverted nanoparticle with an antiferromagnetic core and a ferromagnetic binary alloy shell of the type B_xC_{1-x} by Monte Carlo (MC) simulations. Exchange bias exhibits a non-monotonic behavior with the varying value of the concentration of the type-B magnetic components, x. Coercivity exhibits a monotonic or a non-monotonic variation with x depending on the relative strength between unlike magnetic components in the shell. Also, we have examined the effects of the cooling field process on the magnetic properties of the inverted nanoparticle. Our MC simulation results provide an alternative way for tuning the exchange bias and coercivity of bimagnetic core/shell nanoparticles.

Skyrmion lattice phases in thin film multilayer

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Skyrmions are magnetic whirls realized in ultrathin metal multilayer films. In dilute systems the diffusion of these peculiar micrometer size objects is typically governed by a hopping motion (akin to diffusion in solids) between pinning sites. In denser systems, so-called skyrmion lattices exhibit characteristics of two dimensional behavior. In contrast to previously studied 2d colloidal systems, the skyrmion size and density can be tuned by temperature and magnetic fields. This allows for the system to be driven from a liquid phase to the onset of a hexatic phase as deduced from the analysis of the hexagonal order. Using coarse-grained molecular dynamics simulations of soft disks, the skyrmion interaction potentials are determined, and it is found that the simulations are able to reproduce the phase behavior. This shows that not only the static behavior of skyrmions is qualitatively well described in terms of a simple 2d model system but skyrmion lattices are versatile and tunable systems that allow for studying phases and phase transitions in reduced dimensions.

Scaling of the random-field Ising model in two dimensions

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Being one of the simplest models of magnetic systems with quenched disorder, the random-field Ising model shows surprisingly rich critical behavior. Only recently has it been possible with the help of large-scale numerical

simulations to shed some light on a range of fundamental questions in three and higher dimensions, such as universality, critical scaling and dimensional reduction. The two-dimensional model has received less attention, but is no less fascinating. We solve a long-standing puzzle by presenting compelling numerical evidence for the scaling behavior of the correlation length ξ. Results for two lattice geometries, square and triangular, consistently support the form $\xi \sim \exp[A/h^2]$, where h denotes the random-field strength, in line with early theoretical work [1], but at variance with some more recent numerical and analytical results [2, 3]. We also investigate the more widely used break-up length scale of the system, which we however find to be afflicted by much stronger scaling corrections and hence a rather less useful quantity.

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Simulation of equilibrium and non-equilibrium unfolding and refolding processes for RNA secondary structures (P)

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We study numerically the behavior of RNA secondary structures under influence of a varying external force. An extension of the sampling algorithm of Higgs to the case with external force, which allows us to perfectly sample secondary structures in true equilibrium, is presented. By using this approach, we are able to generate equilibrium unfolding and refolding trajectories. Furthermore, by means of a Monte Carlo sampling of secondary structures, we simulate, starting from equilibrium configurations, fast non-equilibrium unfolding and refolding processes, while measuring the performed work. Using a sophisticated large-deviation algorithm to sample vectors of random numbers, utilized to sample the non-equilibrium trajectories, we can resolve the work distributions with high precision for a medium-size (length $L = 100$) RNA hairpin structure down to probabilities as small as 10^{-46}. By comparison with exact free-energy calculations, we are able to verify the theorems of Crooks and Jarzynski. We compare force-extension curves and the secondary structure configurations during unfolding and refolding, conditioned to selected values of the measured work W, with those of typical equilibrium processes.

Inhomogeneous phases in the Gross-Neveu model

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We present and discuss recent results on the phase diagram of the multiflavour Gross-Neveu model at finite temperature and fermion density. We find a inhomogeneous phase at low temperature and high density. The results for a finite number of fermion species reminds the analytic large N result.

Theory of equilibrium cluster formation in solutions of extended particles

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What determines the size of an equilibrium cluster inside a supercooled solution of extended particles? We present a theory that describes the size of such an equilibrium cluster inside a finite-volume, dilute solution of homopolymers as a stereotypical example of extended particles. Our theory builds on the energetic and entropic considerations introduced [1] and verified [2] for equilibrium particle droplets. We then generalize these

considerations to match the analogy between particle droplets and polymer clusters [3]. In order to constrain all free parameters, we perform finite-size scaling analyses of simulation results from large-scale parallel multicanonical simulations and find that the free parameters do not depend on the degree of polymerization. The result is a leading-order theory that can be fully parameterized with finite-size scaling amplitudes and the asymptotic transition temperature.

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